



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 07:22 PM EST

PDB ID : 1TNV  
Title : CRYSTAL STRUCTURAL ANALYSIS OF TOBACCO NECROSIS VIRUS  
(TNV) AT 5 ANGSTROMS RESOLUTION  
Authors : Tsukihara, T.  
Deposited on : 1994-03-11  
Resolution : 5.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

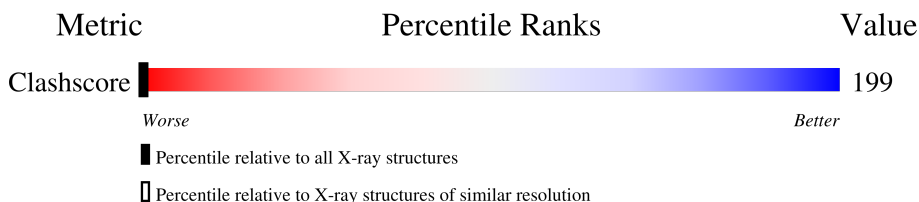
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 5.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric     | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|------------|-----------------------------|---|
| Clashscore | 141614                      | 1000 (6.16-3.82)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 186    |  |
| 1   | B     | 186    |  |
| 2   | C     | 210    |  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2328 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TOBACCO NECROSIS VIRUS (SUBUNIT VP1).

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   |         |         |       |
| 1   | A     | 186      | 744   | 372 | 186 | 186 | 0       | 0       | 0     |
| 1   | B     | 186      | 744   | 372 | 186 | 186 | 0       | 0       | 0     |

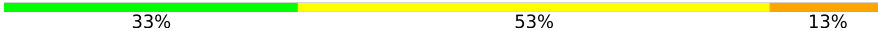
- Molecule 2 is a protein called TOBACCO NECROSIS VIRUS (SUBUNIT VP3).

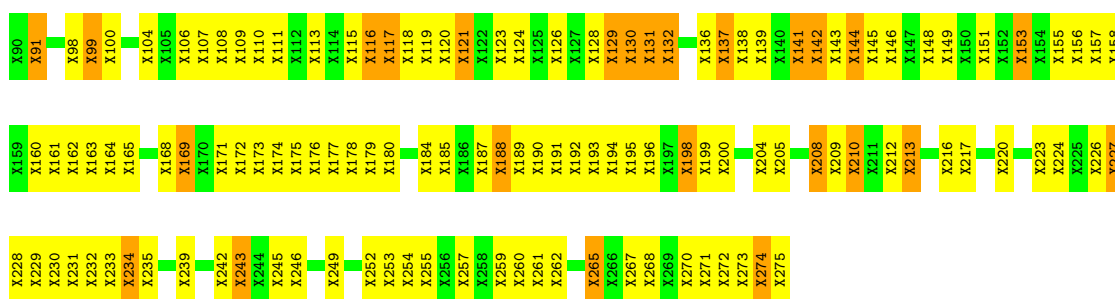
| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   |         |         |       |
| 2   | C     | 210      | 840   | 420 | 210 | 210 | 0       | 0       | 0     |

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

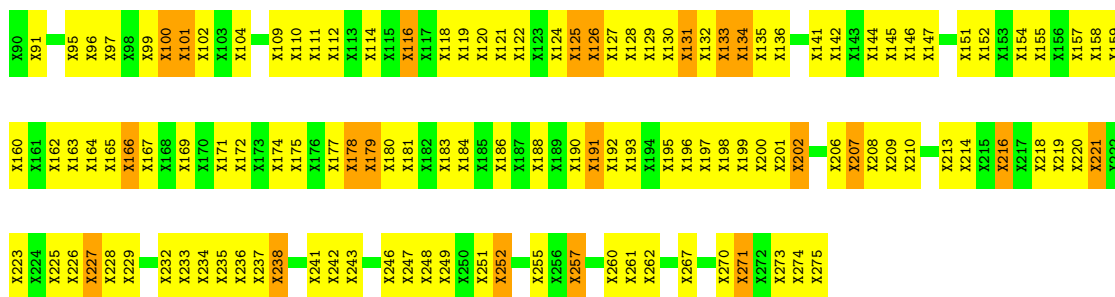
- Molecule 1: TOBACCO NECROSIS VIRUS (SUBUNIT VP1)

Chain A: 



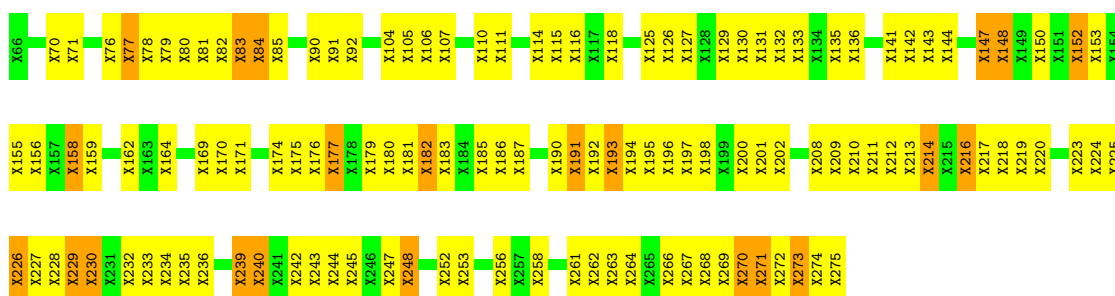
- Molecule 1: TOBACCO NECROSIS VIRUS (SUBUNIT VP1)

Chain B: 



- Molecule 2: TOBACCO NECROSIS VIRUS (SUBUNIT VP3)

Chain C: 



## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 42 3 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 338.00Å 338.00Å 338.00Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | (Not available) – 5.00<br>97.57 – 5.52                       | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) ((Not available)-5.00)<br>42.8 (97.57-5.52)  | Depositor<br>EDS |
| $R_{merge}$   | (Not available)  | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$   | -  | Xtrriage         |
| Refinement program  | NCS  | Depositor        |
| R, $R_{free}$   | (Not available) , (Not available)<br>0.381 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 33.7   | Xtrriage         |
| Anisotropy  | 0.000  | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.16 , 999.0   | EDS              |
| L-test for twinning <sup>1</sup>  | $\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$  | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                       | Xtrriage         |
| $F_o, F_c$ correlation  | 0.68   | EDS              |
| Total number of atoms   | 2328   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 0.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 41                  |
| 1   | B     | 0                   | 49                  |
| 2   | C     | 0                   | 45                  |
| All | All   | 0                   | 135                 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (135) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 106 | UNK  | Mainchain |
| 1   | A     | 113 | UNK  | Mainchain |
| 1   | A     | 116 | UNK  | Mainchain |
| 1   | A     | 117 | UNK  | Mainchain |
| 1   | A     | 121 | UNK  | Mainchain |
| 1   | A     | 129 | UNK  | Mainchain |
| 1   | A     | 130 | UNK  | Mainchain |
| 1   | A     | 131 | UNK  | Mainchain |
| 1   | A     | 132 | UNK  | Mainchain |
| 1   | A     | 137 | UNK  | Mainchain |
| 1   | A     | 141 | UNK  | Mainchain |
| 1   | A     | 142 | UNK  | Mainchain |
| 1   | A     | 144 | UNK  | Mainchain |
| 1   | A     | 145 | UNK  | Mainchain |
| 1   | A     | 146 | UNK  | Mainchain |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 1          | A            | 148        | UNK         | Mainchain    |
| 1          | A            | 149        | UNK         | Mainchain    |
| 1          | A            | 153        | UNK         | Mainchain    |
| 1          | A            | 169        | UNK         | Mainchain    |
| 1          | A            | 180        | UNK         | Mainchain    |
| 1          | A            | 188        | UNK         | Mainchain    |
| 1          | A            | 198        | UNK         | Mainchain    |
| 1          | A            | 199        | UNK         | Mainchain    |
| 1          | A            | 208        | UNK         | Mainchain    |
| 1          | A            | 210        | UNK         | Mainchain    |
| 1          | A            | 213        | UNK         | Mainchain    |
| 1          | A            | 220        | UNK         | Mainchain    |
| 1          | A            | 227        | UNK         | Mainchain    |
| 1          | A            | 229        | UNK         | Mainchain    |
| 1          | A            | 234        | UNK         | Mainchain    |
| 1          | A            | 242        | UNK         | Mainchain    |
| 1          | A            | 243        | UNK         | Mainchain    |
| 1          | A            | 249        | UNK         | Mainchain    |
| 1          | A            | 255        | UNK         | Mainchain    |
| 1          | A            | 257        | UNK         | Mainchain    |
| 1          | A            | 259        | UNK         | Mainchain    |
| 1          | A            | 260        | UNK         | Mainchain    |
| 1          | A            | 265        | UNK         | Mainchain    |
| 1          | A            | 274        | UNK         | Mainchain    |
| 1          | A            | 91         | UNK         | Mainchain    |
| 1          | A            | 99         | UNK         | Mainchain    |
| 1          | B            | 100        | UNK         | Mainchain    |
| 1          | B            | 101        | UNK         | Mainchain    |
| 1          | B            | 111        | UNK         | Peptide      |
| 1          | B            | 112        | UNK         | Mainchain    |
| 1          | B            | 114        | UNK         | Mainchain    |
| 1          | B            | 116        | UNK         | Mainchain    |
| 1          | B            | 121        | UNK         | Mainchain    |
| 1          | B            | 122        | UNK         | Mainchain    |
| 1          | B            | 125        | UNK         | Mainchain    |
| 1          | B            | 126        | UNK         | Mainchain    |
| 1          | B            | 131        | UNK         | Mainchain    |
| 1          | B            | 133        | UNK         | Mainchain    |
| 1          | B            | 134        | UNK         | Mainchain    |
| 1          | B            | 141        | UNK         | Mainchain    |
| 1          | B            | 142        | UNK         | Mainchain    |
| 1          | B            | 145        | UNK         | Mainchain    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 1          | B            | 154        | UNK         | Mainchain    |
| 1          | B            | 155        | UNK         | Mainchain    |
| 1          | B            | 157        | UNK         | Mainchain    |
| 1          | B            | 166        | UNK         | Mainchain    |
| 1          | B            | 169        | UNK         | Mainchain    |
| 1          | B            | 174        | UNK         | Mainchain    |
| 1          | B            | 178        | UNK         | Mainchain    |
| 1          | B            | 179        | UNK         | Mainchain    |
| 1          | B            | 191        | UNK         | Mainchain    |
| 1          | B            | 193        | UNK         | Mainchain    |
| 1          | B            | 202        | UNK         | Mainchain    |
| 1          | B            | 207        | UNK         | Mainchain    |
| 1          | B            | 208        | UNK         | Mainchain    |
| 1          | B            | 213        | UNK         | Mainchain    |
| 1          | B            | 214        | UNK         | Mainchain    |
| 1          | B            | 216        | UNK         | Mainchain    |
| 1          | B            | 221        | UNK         | Mainchain    |
| 1          | B            | 223        | UNK         | Mainchain    |
| 1          | B            | 227        | UNK         | Mainchain    |
| 1          | B            | 232        | UNK         | Mainchain    |
| 1          | B            | 238        | UNK         | Mainchain    |
| 1          | B            | 241        | UNK         | Mainchain    |
| 1          | B            | 243        | UNK         | Mainchain    |
| 1          | B            | 249        | UNK         | Mainchain    |
| 1          | B            | 251        | UNK         | Mainchain    |
| 1          | B            | 252        | UNK         | Mainchain    |
| 1          | B            | 257        | UNK         | Mainchain    |
| 1          | B            | 260        | UNK         | Mainchain    |
| 1          | B            | 261        | UNK         | Mainchain    |
| 1          | B            | 262        | UNK         | Mainchain    |
| 1          | B            | 271        | UNK         | Mainchain    |
| 1          | B            | 91         | UNK         | Mainchain    |
| 1          | B            | 97         | UNK         | Mainchain    |
| 2          | C            | 105        | UNK         | Mainchain    |
| 2          | C            | 107        | UNK         | Mainchain    |
| 2          | C            | 110        | UNK         | Mainchain    |
| 2          | C            | 111        | UNK         | Mainchain    |
| 2          | C            | 118        | UNK         | Mainchain    |
| 2          | C            | 127        | UNK         | Mainchain    |
| 2          | C            | 129        | UNK         | Mainchain    |
| 2          | C            | 130        | UNK         | Mainchain    |
| 2          | C            | 135        | UNK         | Mainchain    |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | C     | 136 | UNK  | Mainchain |
| 2   | C     | 141 | UNK  | Mainchain |
| 2   | C     | 147 | UNK  | Mainchain |
| 2   | C     | 148 | UNK  | Mainchain |
| 2   | C     | 152 | UNK  | Mainchain |
| 2   | C     | 156 | UNK  | Mainchain |
| 2   | C     | 158 | UNK  | Mainchain |
| 2   | C     | 171 | UNK  | Mainchain |
| 2   | C     | 177 | UNK  | Mainchain |
| 2   | C     | 182 | UNK  | Mainchain |
| 2   | C     | 183 | UNK  | Mainchain |
| 2   | C     | 185 | UNK  | Mainchain |
| 2   | C     | 190 | UNK  | Mainchain |
| 2   | C     | 191 | UNK  | Mainchain |
| 2   | C     | 193 | UNK  | Mainchain |
| 2   | C     | 194 | UNK  | Mainchain |
| 2   | C     | 197 | UNK  | Mainchain |
| 2   | C     | 208 | UNK  | Mainchain |
| 2   | C     | 209 | UNK  | Mainchain |
| 2   | C     | 214 | UNK  | Mainchain |
| 2   | C     | 216 | UNK  | Mainchain |
| 2   | C     | 220 | UNK  | Mainchain |
| 2   | C     | 226 | UNK  | Mainchain |
| 2   | C     | 229 | UNK  | Mainchain |
| 2   | C     | 230 | UNK  | Mainchain |
| 2   | C     | 239 | UNK  | Mainchain |
| 2   | C     | 240 | UNK  | Mainchain |
| 2   | C     | 248 | UNK  | Mainchain |
| 2   | C     | 253 | UNK  | Mainchain |
| 2   | C     | 256 | UNK  | Mainchain |
| 2   | C     | 270 | UNK  | Mainchain |
| 2   | C     | 271 | UNK  | Mainchain |
| 2   | C     | 273 | UNK  | Mainchain |
| 2   | C     | 77  | UNK  | Mainchain |
| 2   | C     | 83  | UNK  | Mainchain |
| 2   | C     | 84  | UNK  | Mainchain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 744   | 0        | 53       | 172     | 0            |
| 1   | B     | 744   | 0        | 33       | 153     | 0            |
| 2   | C     | 840   | 0        | 52       | 167     | 0            |
| All | All   | 2328  | 0        | 138      | 491     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 199.

All (491) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 2:C:175:UNK:C  | 2:C:175:UNK:CA | 1.76                     | 1.62              |
| 2:C:266:UNK:C  | 2:C:266:UNK:CA | 1.76                     | 1.62              |
| 1:A:131:UNK:C  | 1:A:131:UNK:CA | 1.76                     | 1.62              |
| 1:A:272:UNK:C  | 1:A:272:UNK:CA | 1.76                     | 1.62              |
| 1:B:270:UNK:C  | 1:B:270:UNK:CA | 1.76                     | 1.62              |
| 1:A:178:UNK:C  | 1:A:178:UNK:CA | 1.76                     | 1.61              |
| 1:A:191:UNK:C  | 1:A:191:UNK:CA | 1.76                     | 1.61              |
| 1:A:275:UNK:C  | 1:A:275:UNK:CA | 1.76                     | 1.61              |
| 1:B:235:UNK:C  | 1:B:235:UNK:CA | 1.76                     | 1.61              |
| 2:C:201:UNK:C  | 2:C:201:UNK:CA | 1.76                     | 1.60              |
| 1:B:146:UNK:C  | 1:B:146:UNK:CA | 1.76                     | 1.58              |
| 1:A:267:UNK:C  | 1:A:267:UNK:CA | 1.76                     | 1.58              |
| 1:B:133:UNK:C  | 1:B:133:UNK:CA | 1.76                     | 1.58              |
| 1:B:246:UNK:C  | 1:B:246:UNK:CA | 1.76                     | 1.58              |
| 2:C:79:UNK:C   | 2:C:79:UNK:CA  | 1.76                     | 1.58              |
| 2:C:217:UNK:C  | 2:C:217:UNK:CA | 1.76                     | 1.58              |
| 2:C:229:UNK:C  | 2:C:229:UNK:CA | 1.76                     | 1.58              |
| 2:C:261:UNK:C  | 2:C:261:UNK:CA | 1.76                     | 1.58              |
| 1:A:253:UNK:C  | 1:A:253:UNK:CA | 1.76                     | 1.57              |
| 1:B:201:UNK:C  | 1:B:201:UNK:CA | 1.82                     | 1.57              |
| 2:C:174:UNK:C  | 2:C:174:UNK:CA | 1.82                     | 1.57              |
| 1:A:274:UNK:C  | 1:A:274:UNK:CA | 1.82                     | 1.56              |
| 2:C:180:UNK:C  | 2:C:180:UNK:CA | 1.82                     | 1.56              |
| 2:C:264:UNK:C  | 2:C:264:UNK:CA | 1.82                     | 1.56              |
| 1:A:129:UNK:C  | 1:A:129:UNK:CA | 1.76                     | 1.56              |
| 2:C:235:UNK:C  | 2:C:235:UNK:CA | 1.76                     | 1.55              |
| 1:A:245:UNK:C  | 1:A:245:UNK:CA | 1.82                     | 1.55              |
| 2:C:143:UNK:C  | 2:C:143:UNK:CA | 1.82                     | 1.55              |
| 2:C:219:UNK:CA | 2:C:219:UNK:N  | 1.69                     | 1.55              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:B:99:UNK:C   | 1:B:99:UNK:CA  | 1.76                     | 1.55              |
| 2:C:78:UNK:N   | 2:C:78:UNK:CA  | 1.69                     | 1.55              |
| 2:C:233:UNK:C  | 2:C:233:UNK:CA | 1.82                     | 1.54              |
| 1:B:95:UNK:C   | 1:B:95:UNK:CA  | 1.82                     | 1.54              |
| 1:A:174:UNK:CA | 1:A:174:UNK:N  | 1.69                     | 1.54              |
| 1:A:232:UNK:C  | 1:A:232:UNK:CA | 1.85                     | 1.54              |
| 1:B:206:UNK:C  | 1:B:206:UNK:CA | 1.82                     | 1.54              |
| 1:B:210:UNK:N  | 1:B:210:UNK:CA | 1.69                     | 1.54              |
| 1:B:238:UNK:N  | 1:B:238:UNK:CA | 1.69                     | 1.54              |
| 2:C:170:UNK:CA | 2:C:170:UNK:N  | 1.69                     | 1.54              |
| 2:C:187:UNK:N  | 2:C:187:UNK:CA | 1.69                     | 1.54              |
| 2:C:225:UNK:CA | 2:C:225:UNK:N  | 1.69                     | 1.53              |
| 2:C:90:UNK:C   | 2:C:90:UNK:CA  | 1.85                     | 1.53              |
| 2:C:132:UNK:C  | 2:C:132:UNK:CA | 1.82                     | 1.53              |
| 1:B:110:UNK:N  | 1:B:110:UNK:CA | 1.72                     | 1.53              |
| 1:B:101:UNK:C  | 1:B:101:UNK:CA | 1.82                     | 1.52              |
| 1:A:227:UNK:N  | 1:A:227:UNK:CA | 1.69                     | 1.52              |
| 1:B:274:UNK:N  | 1:B:274:UNK:CA | 1.69                     | 1.52              |
| 2:C:77:UNK:N   | 2:C:77:UNK:CA  | 1.69                     | 1.52              |
| 1:A:213:UNK:N  | 1:A:213:UNK:CA | 1.69                     | 1.52              |
| 1:B:191:UNK:N  | 1:B:191:UNK:CA | 1.72                     | 1.52              |
| 2:C:126:UNK:N  | 2:C:126:UNK:CA | 1.69                     | 1.52              |
| 1:B:160:UNK:N  | 1:B:160:UNK:CA | 1.69                     | 1.52              |
| 2:C:131:UNK:C  | 2:C:131:UNK:CA | 1.82                     | 1.52              |
| 1:A:155:UNK:C  | 1:A:155:UNK:CA | 1.82                     | 1.52              |
| 1:A:157:UNK:C  | 1:A:157:UNK:CA | 1.82                     | 1.52              |
| 1:A:231:UNK:N  | 1:A:231:UNK:CA | 1.69                     | 1.52              |
| 1:B:179:UNK:N  | 1:B:179:UNK:CA | 1.69                     | 1.52              |
| 1:A:99:UNK:CA  | 1:A:99:UNK:N   | 1.72                     | 1.51              |
| 1:A:196:UNK:N  | 1:A:196:UNK:CA | 1.69                     | 1.51              |
| 2:C:210:UNK:CA | 2:C:210:UNK:C  | 1.82                     | 1.51              |
| 1:B:172:UNK:N  | 1:B:172:UNK:CA | 1.72                     | 1.51              |
| 1:B:178:UNK:N  | 1:B:178:UNK:CA | 1.72                     | 1.51              |
| 1:A:162:UNK:N  | 1:A:162:UNK:CA | 1.72                     | 1.51              |
| 1:B:135:UNK:C  | 1:B:135:UNK:CA | 1.85                     | 1.51              |
| 1:B:228:UNK:C  | 1:B:228:UNK:CA | 1.85                     | 1.51              |
| 2:C:82:UNK:N   | 2:C:82:UNK:CA  | 1.72                     | 1.51              |
| 1:A:205:UNK:N  | 1:A:205:UNK:CA | 1.69                     | 1.51              |
| 1:A:209:UNK:N  | 1:A:209:UNK:CA | 1.72                     | 1.51              |
| 1:A:233:UNK:N  | 1:A:233:UNK:CA | 1.72                     | 1.51              |
| 1:A:143:UNK:N  | 1:A:143:UNK:CA | 1.72                     | 1.50              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:169:UNK:N  | 1:A:169:UNK:CA | 1.72                     | 1.50              |
| 2:C:71:UNK:N   | 2:C:71:UNK:CA  | 1.72                     | 1.50              |
| 1:A:194:UNK:N  | 1:A:194:UNK:CA | 1.69                     | 1.50              |
| 1:B:167:UNK:N  | 1:B:167:UNK:CA | 1.72                     | 1.49              |
| 1:B:181:UNK:N  | 1:B:181:UNK:CA | 1.72                     | 1.49              |
| 2:C:235:UNK:CA | 2:C:235:UNK:N  | 1.72                     | 1.49              |
| 2:C:245:UNK:N  | 2:C:245:UNK:CA | 1.76                     | 1.49              |
| 1:A:108:UNK:N  | 1:A:108:UNK:CA | 1.72                     | 1.49              |
| 2:C:84:UNK:N   | 2:C:84:UNK:CA  | 1.76                     | 1.49              |
| 2:C:153:UNK:N  | 2:C:153:UNK:CA | 1.72                     | 1.49              |
| 2:C:159:UNK:N  | 2:C:159:UNK:CA | 1.76                     | 1.49              |
| 1:B:163:UNK:N  | 1:B:163:UNK:CA | 1.72                     | 1.49              |
| 1:B:237:UNK:N  | 1:B:237:UNK:CA | 1.72                     | 1.49              |
| 1:A:110:UNK:N  | 1:A:110:UNK:CA | 1.72                     | 1.48              |
| 1:A:271:UNK:N  | 1:A:271:UNK:CA | 1.72                     | 1.48              |
| 1:B:229:UNK:N  | 1:B:229:UNK:CA | 1.72                     | 1.48              |
| 2:C:263:UNK:N  | 2:C:263:UNK:CA | 1.72                     | 1.48              |
| 1:B:129:UNK:N  | 1:B:129:UNK:CA | 1.76                     | 1.48              |
| 1:B:152:UNK:N  | 1:B:152:UNK:CA | 1.72                     | 1.48              |
| 1:B:199:UNK:N  | 1:B:199:UNK:CA | 1.72                     | 1.48              |
| 2:C:273:UNK:N  | 2:C:273:UNK:CA | 1.72                     | 1.48              |
| 1:B:120:UNK:N  | 1:B:120:UNK:CA | 1.72                     | 1.47              |
| 1:B:125:UNK:N  | 1:B:125:UNK:CA | 1.72                     | 1.47              |
| 1:B:196:UNK:N  | 1:B:196:UNK:CA | 1.76                     | 1.47              |
| 1:B:198:UNK:N  | 1:B:198:UNK:CA | 1.72                     | 1.47              |
| 1:A:217:UNK:N  | 1:A:217:UNK:CA | 1.72                     | 1.47              |
| 2:C:214:UNK:N  | 2:C:214:UNK:CA | 1.72                     | 1.47              |
| 2:C:240:UNK:N  | 2:C:240:UNK:CA | 1.76                     | 1.47              |
| 2:C:116:UNK:CA | 2:C:116:UNK:N  | 1.76                     | 1.47              |
| 1:A:189:UNK:CA | 1:A:189:UNK:N  | 1.76                     | 1.46              |
| 1:B:184:UNK:N  | 1:B:184:UNK:CA | 1.72                     | 1.46              |
| 1:A:161:UNK:N  | 1:A:161:UNK:CA | 1.72                     | 1.46              |
| 1:A:163:UNK:N  | 1:A:163:UNK:CA | 1.76                     | 1.44              |
| 2:C:91:UNK:N   | 2:C:91:UNK:CA  | 1.82                     | 1.42              |
| 1:A:164:UNK:N  | 1:A:164:UNK:CA | 1.82                     | 1.41              |
| 1:B:131:UNK:N  | 1:B:131:UNK:CA | 1.82                     | 1.40              |
| 1:A:142:UNK:N  | 1:A:142:UNK:CA | 1.82                     | 1.40              |
| 2:C:198:UNK:O  | 2:C:200:UNK:N  | 1.66                     | 1.28              |
| 1:B:134:UNK:N  | 1:B:219:UNK:O  | 1.76                     | 1.19              |
| 1:A:137:UNK:N  | 1:A:262:UNK:O  | 1.82                     | 1.13              |
| 1:B:183:UNK:C  | 1:B:184:UNK:CA | 2.27                     | 1.13              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:157:UNK:C  | 1:A:157:UNK:O  | 0.83                     | 1.13              |
| 1:B:270:UNK:O  | 1:B:273:UNK:N  | 1.82                     | 1.12              |
| 2:C:242:UNK:C  | 2:C:242:UNK:O  | 0.83                     | 1.12              |
| 1:A:188:UNK:O  | 1:A:190:UNK:N  | 1.82                     | 1.11              |
| 1:B:128:UNK:C  | 1:B:129:UNK:CA | 2.29                     | 1.09              |
| 1:A:109:UNK:C  | 1:A:110:UNK:CA | 2.34                     | 1.04              |
| 2:C:191:UNK:C  | 2:C:193:UNK:H2 | 1.68                     | 1.02              |
| 1:A:226:UNK:C  | 1:A:227:UNK:CA | 2.39                     | 1.01              |
| 2:C:76:UNK:C   | 2:C:77:UNK:CA  | 2.39                     | 1.01              |
| 1:A:216:UNK:C  | 1:A:217:UNK:CA | 2.39                     | 1.00              |
| 2:C:175:UNK:CA | 2:C:176:UNK:N  | 2.24                     | 1.00              |
| 1:A:195:UNK:C  | 1:A:196:UNK:CA | 2.39                     | 1.00              |
| 2:C:153:UNK:CA | 2:C:247:UNK:CA | 2.39                     | 0.99              |
| 1:B:177:UNK:C  | 1:B:178:UNK:CA | 2.41                     | 0.98              |
| 1:B:246:UNK:CA | 1:B:247:UNK:N  | 2.27                     | 0.98              |
| 1:A:198:UNK:O  | 1:A:200:UNK:N  | 1.97                     | 0.97              |
| 1:B:101:UNK:CA | 1:B:102:UNK:N  | 2.27                     | 0.97              |
| 1:B:178:UNK:C  | 1:B:179:UNK:CA | 2.41                     | 0.97              |
| 2:C:77:UNK:C   | 2:C:78:UNK:CA  | 2.41                     | 0.97              |
| 2:C:90:UNK:CA  | 2:C:91:UNK:N   | 2.29                     | 0.95              |
| 2:C:218:UNK:C  | 2:C:219:UNK:CA | 2.44                     | 0.95              |
| 2:C:271:UNK:C  | 2:C:273:UNK:N  | 2.29                     | 0.95              |
| 1:A:129:UNK:CA | 1:A:130:UNK:N  | 2.29                     | 0.95              |
| 2:C:273:UNK:O  | 2:C:275:UNK:N  | 2.00                     | 0.94              |
| 1:B:120:UNK:N  | 1:B:120:UNK:C  | 2.29                     | 0.94              |
| 2:C:261:UNK:CA | 2:C:262:UNK:N  | 2.29                     | 0.94              |
| 1:A:120:UNK:O  | 1:A:121:UNK:O  | 1.85                     | 0.94              |
| 2:C:242:UNK:O  | 2:C:243:UNK:N  | 2.00                     | 0.94              |
| 1:A:253:UNK:C  | 1:A:253:UNK:N  | 2.29                     | 0.93              |
| 1:A:141:UNK:C  | 1:A:142:UNK:CA | 2.46                     | 0.93              |
| 2:C:152:UNK:C  | 2:C:153:UNK:CA | 2.46                     | 0.93              |
| 2:C:272:UNK:C  | 2:C:273:UNK:CA | 2.46                     | 0.93              |
| 2:C:213:UNK:C  | 2:C:214:UNK:CA | 2.46                     | 0.92              |
| 1:B:228:UNK:C  | 1:B:229:UNK:CA | 2.48                     | 0.91              |
| 1:B:236:UNK:C  | 1:B:237:UNK:CA | 2.48                     | 0.91              |
| 1:A:232:UNK:C  | 1:A:233:UNK:CA | 2.48                     | 0.91              |
| 1:B:238:UNK:N  | 1:B:238:UNK:C  | 2.34                     | 0.91              |
| 1:A:157:UNK:O  | 1:A:158:UNK:N  | 2.03                     | 0.90              |
| 1:A:160:UNK:C  | 1:A:161:UNK:CA | 2.48                     | 0.90              |
| 1:A:161:UNK:C  | 1:A:162:UNK:CA | 2.48                     | 0.90              |
| 2:C:224:UNK:C  | 2:C:225:UNK:CA | 2.48                     | 0.89              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:B:198:UNK:O  | 1:B:200:UNK:N  | 2.06                     | 0.89              |
| 2:C:271:UNK:O  | 2:C:273:UNK:N  | 2.06                     | 0.89              |
| 2:C:131:UNK:CA | 2:C:132:UNK:N  | 2.37                     | 0.88              |
| 2:C:214:UNK:N  | 2:C:214:UNK:C  | 2.37                     | 0.88              |
| 1:A:275:UNK:C  | 1:A:275:UNK:N  | 2.37                     | 0.88              |
| 1:B:152:UNK:N  | 1:B:152:UNK:C  | 2.37                     | 0.87              |
| 1:A:107:UNK:C  | 1:A:108:UNK:CA | 2.53                     | 0.86              |
| 1:A:270:UNK:C  | 1:A:271:UNK:CA | 2.53                     | 0.86              |
| 1:A:267:UNK:CA | 1:A:268:UNK:N  | 2.39                     | 0.86              |
| 1:B:119:UNK:C  | 1:B:120:UNK:CA | 2.53                     | 0.86              |
| 1:B:198:UNK:N  | 1:B:198:UNK:C  | 2.39                     | 0.86              |
| 2:C:180:UNK:C  | 2:C:180:UNK:N  | 2.39                     | 0.85              |
| 1:A:232:UNK:N  | 1:A:233:UNK:N  | 2.24                     | 0.85              |
| 1:B:246:UNK:C  | 1:B:246:UNK:N  | 2.39                     | 0.85              |
| 2:C:115:UNK:C  | 2:C:116:UNK:CA | 2.53                     | 0.85              |
| 2:C:239:UNK:C  | 2:C:240:UNK:CA | 2.53                     | 0.85              |
| 1:B:160:UNK:N  | 1:B:160:UNK:C  | 2.39                     | 0.85              |
| 2:C:229:UNK:C  | 2:C:229:UNK:N  | 2.39                     | 0.85              |
| 1:A:157:UNK:C  | 1:A:157:UNK:N  | 2.39                     | 0.85              |
| 1:A:232:UNK:C  | 1:A:232:UNK:N  | 2.39                     | 0.85              |
| 1:B:146:UNK:C  | 1:B:146:UNK:N  | 2.39                     | 0.84              |
| 1:B:270:UNK:CA | 1:B:271:UNK:N  | 2.39                     | 0.84              |
| 1:A:232:UNK:CA | 1:A:233:UNK:N  | 2.39                     | 0.84              |
| 2:C:82:UNK:N   | 2:C:82:UNK:C   | 2.39                     | 0.84              |
| 1:A:188:UNK:C  | 1:A:189:UNK:CA | 2.55                     | 0.83              |
| 1:A:209:UNK:N  | 1:A:209:UNK:C  | 2.41                     | 0.83              |
| 1:A:230:UNK:C  | 1:A:231:UNK:CA | 2.48                     | 0.83              |
| 1:B:159:UNK:C  | 1:B:160:UNK:CA | 2.55                     | 0.83              |
| 2:C:169:UNK:C  | 2:C:170:UNK:CA | 2.53                     | 0.83              |
| 2:C:235:UNK:CA | 2:C:236:UNK:N  | 2.41                     | 0.83              |
| 1:A:174:UNK:N  | 1:A:174:UNK:C  | 2.39                     | 0.83              |
| 1:A:188:UNK:C  | 1:A:190:UNK:N  | 2.41                     | 0.83              |
| 1:B:228:UNK:CA | 1:B:229:UNK:N  | 2.39                     | 0.83              |
| 2:C:201:UNK:C  | 2:C:201:UNK:N  | 2.41                     | 0.82              |
| 1:B:95:UNK:CA  | 1:B:96:UNK:N   | 2.41                     | 0.82              |
| 1:A:193:UNK:C  | 1:A:194:UNK:CA | 2.57                     | 0.82              |
| 1:A:208:UNK:C  | 1:A:209:UNK:CA | 2.57                     | 0.82              |
| 1:B:195:UNK:C  | 1:B:196:UNK:CA | 2.53                     | 0.81              |
| 1:B:237:UNK:C  | 1:B:238:UNK:CA | 2.57                     | 0.81              |
| 2:C:233:UNK:CA | 2:C:234:UNK:N  | 2.41                     | 0.81              |
| 1:B:216:UNK:C  | 1:B:218:UNK:H  | 1.91                     | 0.81              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:B:99:UNK:CA  | 1:B:100:UNK:N  | 2.37                     | 0.81              |
| 2:C:266:UNK:CA | 2:C:267:UNK:N  | 2.41                     | 0.81              |
| 1:B:99:UNK:C   | 1:B:99:UNK:N   | 2.44                     | 0.81              |
| 1:B:152:UNK:O  | 1:B:248:UNK:N  | 2.14                     | 0.81              |
| 2:C:242:UNK:O  | 2:C:242:UNK:CA | 2.29                     | 0.81              |
| 1:A:168:UNK:C  | 1:A:169:UNK:CA | 2.60                     | 0.80              |
| 1:B:274:UNK:O  | 1:B:275:UNK:C  | 2.27                     | 0.80              |
| 1:B:184:UNK:N  | 1:B:184:UNK:C  | 2.46                     | 0.79              |
| 1:A:226:UNK:C  | 1:A:227:UNK:C  | 2.60                     | 0.79              |
| 2:C:158:UNK:C  | 2:C:159:UNK:CA | 2.60                     | 0.79              |
| 2:C:219:UNK:N  | 2:C:219:UNK:C  | 2.46                     | 0.79              |
| 2:C:104:UNK:O  | 2:C:252:UNK:O  | 2.00                     | 0.79              |
| 1:B:198:UNK:C  | 1:B:199:UNK:CA | 2.60                     | 0.78              |
| 2:C:79:UNK:CA  | 2:C:80:UNK:N   | 2.46                     | 0.78              |
| 2:C:143:UNK:CA | 2:C:144:UNK:N  | 2.46                     | 0.78              |
| 1:A:173:UNK:C  | 1:A:174:UNK:CA | 2.60                     | 0.78              |
| 2:C:273:UNK:N  | 2:C:273:UNK:C  | 2.46                     | 0.78              |
| 2:C:210:UNK:O  | 2:C:213:UNK:N  | 2.16                     | 0.77              |
| 1:B:273:UNK:C  | 1:B:274:UNK:CA | 2.60                     | 0.77              |
| 2:C:131:UNK:C  | 2:C:131:UNK:N  | 2.48                     | 0.77              |
| 1:B:274:UNK:N  | 1:B:274:UNK:C  | 2.48                     | 0.76              |
| 2:C:217:UNK:CA | 2:C:218:UNK:N  | 2.46                     | 0.76              |
| 1:A:204:UNK:C  | 1:A:205:UNK:CA | 2.60                     | 0.76              |
| 1:A:272:UNK:CA | 1:A:273:UNK:N  | 2.46                     | 0.76              |
| 1:B:163:UNK:N  | 1:B:163:UNK:C  | 2.48                     | 0.76              |
| 2:C:191:UNK:C  | 2:C:193:UNK:N  | 2.46                     | 0.76              |
| 2:C:79:UNK:CA  | 2:C:79:UNK:O   | 2.29                     | 0.76              |
| 1:A:245:UNK:CA | 1:A:246:UNK:N  | 2.48                     | 0.76              |
| 2:C:143:UNK:C  | 2:C:143:UNK:N  | 2.48                     | 0.76              |
| 2:C:174:UNK:CA | 2:C:175:UNK:N  | 2.39                     | 0.76              |
| 1:A:169:UNK:N  | 1:A:169:UNK:C  | 2.48                     | 0.76              |
| 1:B:167:UNK:N  | 1:B:167:UNK:C  | 2.46                     | 0.76              |
| 1:A:189:UNK:N  | 1:A:189:UNK:C  | 2.48                     | 0.75              |
| 1:A:232:UNK:C  | 1:A:234:UNK:N  | 2.48                     | 0.75              |
| 2:C:90:UNK:C   | 2:C:90:UNK:N   | 2.48                     | 0.75              |
| 1:A:171:UNK:O  | 1:A:175:UNK:N  | 2.19                     | 0.75              |
| 1:B:95:UNK:C   | 1:B:95:UNK:N   | 2.48                     | 0.75              |
| 1:B:133:UNK:CA | 1:B:220:UNK:CA | 2.64                     | 0.75              |
| 2:C:186:UNK:C  | 2:C:187:UNK:CA | 2.64                     | 0.74              |
| 2:C:217:UNK:C  | 2:C:217:UNK:N  | 2.48                     | 0.74              |
| 2:C:210:UNK:CA | 2:C:211:UNK:N  | 2.48                     | 0.74              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 2:C:83:UNK:C   | 2:C:84:UNK:CA  | 2.64                     | 0.74              |
| 1:A:178:UNK:CA | 1:A:179:UNK:N  | 2.48                     | 0.74              |
| 1:A:227:UNK:N  | 1:A:227:UNK:C  | 2.48                     | 0.74              |
| 1:A:188:UNK:C  | 1:A:189:UNK:C  | 2.66                     | 0.74              |
| 1:A:162:UNK:O  | 1:A:165:UNK:N  | 2.22                     | 0.73              |
| 2:C:90:UNK:C   | 2:C:91:UNK:CA  | 2.64                     | 0.73              |
| 1:A:91:UNK:O   | 1:A:265:UNK:N  | 2.22                     | 0.73              |
| 1:B:151:UNK:C  | 1:B:152:UNK:CA | 2.60                     | 0.73              |
| 1:B:119:UNK:C  | 1:B:120:UNK:C  | 2.66                     | 0.73              |
| 1:A:142:UNK:C  | 1:A:143:UNK:CA | 2.64                     | 0.72              |
| 1:B:135:UNK:C  | 1:B:135:UNK:N  | 2.48                     | 0.72              |
| 1:A:163:UNK:C  | 1:A:164:UNK:CA | 2.66                     | 0.72              |
| 1:A:162:UNK:C  | 1:A:163:UNK:CA | 2.66                     | 0.72              |
| 1:A:98:UNK:C   | 1:A:99:UNK:CA  | 2.66                     | 0.72              |
| 1:B:166:UNK:C  | 1:B:167:UNK:CA | 2.66                     | 0.72              |
| 2:C:244:UNK:C  | 2:C:245:UNK:CA | 2.64                     | 0.72              |
| 1:B:270:UNK:O  | 1:B:273:UNK:CA | 2.37                     | 0.72              |
| 1:A:155:UNK:C  | 1:A:155:UNK:N  | 2.48                     | 0.72              |
| 1:A:99:UNK:N   | 1:A:99:UNK:C   | 2.53                     | 0.71              |
| 1:A:155:UNK:CA | 1:A:156:UNK:N  | 2.48                     | 0.71              |
| 1:A:213:UNK:N  | 1:A:213:UNK:C  | 2.53                     | 0.71              |
| 2:C:174:UNK:C  | 2:C:174:UNK:N  | 2.48                     | 0.71              |
| 2:C:187:UNK:N  | 2:C:187:UNK:C  | 2.48                     | 0.71              |
| 1:A:267:UNK:C  | 1:A:267:UNK:N  | 2.53                     | 0.71              |
| 1:A:99:UNK:O   | 1:A:100:UNK:O  | 2.08                     | 0.71              |
| 1:B:181:UNK:N  | 1:B:181:UNK:C  | 2.53                     | 0.70              |
| 1:B:233:UNK:O  | 1:B:236:UNK:N  | 2.24                     | 0.70              |
| 2:C:125:UNK:C  | 2:C:126:UNK:CA | 2.64                     | 0.70              |
| 1:A:131:UNK:CA | 1:A:131:UNK:O  | 2.37                     | 0.70              |
| 1:A:172:UNK:O  | 1:A:173:UNK:C  | 2.39                     | 0.70              |
| 1:A:119:UNK:O  | 1:A:120:UNK:C  | 2.39                     | 0.70              |
| 2:C:84:UNK:N   | 2:C:84:UNK:C   | 2.53                     | 0.70              |
| 1:A:129:UNK:C  | 1:A:129:UNK:N  | 2.53                     | 0.70              |
| 1:B:133:UNK:C  | 1:B:133:UNK:N  | 2.53                     | 0.70              |
| 1:B:190:UNK:C  | 1:B:191:UNK:CA | 2.57                     | 0.70              |
| 1:A:142:UNK:N  | 1:A:142:UNK:C  | 2.55                     | 0.69              |
| 1:A:217:UNK:N  | 1:A:217:UNK:C  | 2.53                     | 0.69              |
| 1:B:191:UNK:N  | 1:B:191:UNK:C  | 2.55                     | 0.69              |
| 1:B:144:UNK:O  | 1:B:255:UNK:CA | 2.39                     | 0.69              |
| 1:B:206:UNK:CA | 1:B:207:UNK:N  | 2.55                     | 0.69              |
| 2:C:201:UNK:CA | 2:C:202:UNK:N  | 2.48                     | 0.69              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:253:UNK:CA | 1:A:254:UNK:N  | 2.55                     | 0.68              |
| 1:A:123:UNK:O  | 1:A:126:UNK:N  | 2.27                     | 0.68              |
| 1:A:115:UNK:N  | 1:A:239:UNK:O  | 2.27                     | 0.68              |
| 1:A:139:UNK:O  | 1:A:209:UNK:N  | 2.27                     | 0.68              |
| 1:B:196:UNK:N  | 1:B:196:UNK:C  | 2.55                     | 0.68              |
| 2:C:228:UNK:O  | 2:C:229:UNK:C  | 2.41                     | 0.68              |
| 1:B:124:UNK:C  | 1:B:125:UNK:CA | 2.66                     | 0.68              |
| 1:A:232:UNK:O  | 1:A:234:UNK:N  | 2.27                     | 0.68              |
| 1:B:134:UNK:O  | 1:B:219:UNK:N  | 2.27                     | 0.68              |
| 1:A:274:UNK:C  | 1:A:274:UNK:N  | 2.53                     | 0.68              |
| 1:B:235:UNK:CA | 1:B:236:UNK:N  | 2.48                     | 0.68              |
| 2:C:177:UNK:O  | 2:C:179:UNK:N  | 2.27                     | 0.68              |
| 1:A:132:UNK:N  | 1:A:267:UNK:O  | 2.27                     | 0.68              |
| 1:A:153:UNK:O  | 1:A:185:UNK:N  | 2.27                     | 0.67              |
| 1:B:146:UNK:CA | 1:B:147:UNK:N  | 2.48                     | 0.67              |
| 1:A:195:UNK:C  | 1:A:196:UNK:C  | 2.73                     | 0.67              |
| 1:B:180:UNK:C  | 1:B:181:UNK:CA | 2.64                     | 0.66              |
| 2:C:78:UNK:N   | 2:C:78:UNK:C   | 2.55                     | 0.66              |
| 2:C:233:UNK:C  | 2:C:235:UNK:N  | 2.55                     | 0.66              |
| 1:B:225:UNK:O  | 1:B:226:UNK:C  | 2.41                     | 0.66              |
| 1:B:130:UNK:C  | 1:B:131:UNK:CA | 2.75                     | 0.65              |
| 2:C:132:UNK:CA | 2:C:133:UNK:N  | 2.57                     | 0.65              |
| 2:C:228:UNK:C  | 2:C:229:UNK:C  | 2.75                     | 0.65              |
| 1:A:110:UNK:N  | 1:A:110:UNK:C  | 2.55                     | 0.65              |
| 2:C:155:UNK:O  | 2:C:182:UNK:CA | 2.44                     | 0.65              |
| 1:B:171:UNK:O  | 1:B:175:UNK:N  | 2.29                     | 0.65              |
| 1:B:132:UNK:O  | 1:B:221:UNK:N  | 2.29                     | 0.65              |
| 1:A:194:UNK:N  | 1:A:194:UNK:C  | 2.60                     | 0.65              |
| 1:B:237:UNK:N  | 1:B:237:UNK:C  | 2.60                     | 0.65              |
| 2:C:213:UNK:C  | 2:C:214:UNK:C  | 2.75                     | 0.65              |
| 2:C:262:UNK:C  | 2:C:263:UNK:CA | 2.75                     | 0.65              |
| 1:A:99:UNK:C   | 1:A:100:UNK:O  | 2.39                     | 0.65              |
| 1:A:143:UNK:N  | 1:A:143:UNK:C  | 2.55                     | 0.64              |
| 2:C:79:UNK:C   | 2:C:79:UNK:N   | 2.60                     | 0.64              |
| 1:A:274:UNK:O  | 1:A:275:UNK:C  | 2.46                     | 0.64              |
| 1:A:129:UNK:N  | 1:A:130:UNK:N  | 2.46                     | 0.64              |
| 1:A:191:UNK:O  | 1:A:192:UNK:O  | 2.16                     | 0.64              |
| 2:C:198:UNK:C  | 2:C:200:UNK:N  | 2.60                     | 0.64              |
| 1:B:172:UNK:N  | 1:B:172:UNK:C  | 2.60                     | 0.63              |
| 1:A:91:UNK:N   | 1:A:265:UNK:O  | 2.27                     | 0.63              |
| 2:C:193:UNK:O  | 2:C:198:UNK:O  | 2.16                     | 0.63              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:131:UNK:CA | 1:A:132:UNK:N  | 2.46                     | 0.63              |
| 2:C:106:UNK:CA | 2:C:248:UNK:CA | 2.77                     | 0.63              |
| 1:B:183:UNK:C  | 1:B:184:UNK:C  | 2.75                     | 0.63              |
| 1:B:128:UNK:C  | 1:B:129:UNK:C  | 2.77                     | 0.62              |
| 2:C:91:UNK:N   | 2:C:91:UNK:C   | 2.60                     | 0.62              |
| 2:C:263:UNK:N  | 2:C:263:UNK:C  | 2.60                     | 0.62              |
| 2:C:264:UNK:CA | 2:C:264:UNK:O  | 2.41                     | 0.62              |
| 2:C:217:UNK:N  | 2:C:218:UNK:N  | 2.48                     | 0.61              |
| 1:B:146:UNK:N  | 1:B:147:UNK:N  | 2.46                     | 0.61              |
| 2:C:266:UNK:CA | 2:C:266:UNK:O  | 2.37                     | 0.61              |
| 1:B:201:UNK:CA | 1:B:201:UNK:O  | 2.39                     | 0.61              |
| 1:A:162:UNK:C  | 1:A:164:UNK:N  | 2.64                     | 0.61              |
| 2:C:232:UNK:O  | 2:C:235:UNK:N  | 2.34                     | 0.61              |
| 1:A:274:UNK:C  | 1:A:275:UNK:C  | 2.79                     | 0.61              |
| 1:B:178:UNK:N  | 1:B:178:UNK:C  | 2.64                     | 0.60              |
| 1:B:151:UNK:C  | 1:B:152:UNK:C  | 2.79                     | 0.60              |
| 1:B:233:UNK:O  | 1:B:234:UNK:C  | 2.48                     | 0.60              |
| 1:B:104:UNK:O  | 1:B:252:UNK:CA | 2.48                     | 0.60              |
| 2:C:70:UNK:C   | 2:C:71:UNK:CA  | 2.75                     | 0.60              |
| 1:B:135:UNK:CA | 1:B:136:UNK:N  | 2.64                     | 0.60              |
| 2:C:170:UNK:N  | 2:C:170:UNK:C  | 2.55                     | 0.60              |
| 1:A:108:UNK:N  | 1:A:108:UNK:C  | 2.60                     | 0.60              |
| 1:A:144:UNK:O  | 1:A:187:UNK:O  | 2.19                     | 0.59              |
| 1:A:232:UNK:C  | 1:A:233:UNK:C  | 2.81                     | 0.59              |
| 1:A:157:UNK:CA | 1:A:158:UNK:N  | 2.60                     | 0.59              |
| 2:C:174:UNK:C  | 2:C:176:UNK:N  | 2.66                     | 0.59              |
| 1:A:119:UNK:O  | 1:A:121:UNK:N  | 2.37                     | 0.58              |
| 2:C:216:UNK:C  | 2:C:218:UNK:N  | 2.66                     | 0.58              |
| 1:A:162:UNK:N  | 1:A:162:UNK:C  | 2.66                     | 0.58              |
| 2:C:133:UNK:O  | 2:C:266:UNK:N  | 2.37                     | 0.58              |
| 1:A:198:UNK:C  | 1:A:200:UNK:N  | 2.64                     | 0.58              |
| 2:C:198:UNK:O  | 2:C:200:UNK:CA | 2.48                     | 0.58              |
| 1:B:116:UNK:C  | 1:B:118:UNK:N  | 2.66                     | 0.58              |
| 1:A:151:UNK:O  | 1:A:153:UNK:N  | 2.37                     | 0.58              |
| 2:C:261:UNK:CA | 2:C:261:UNK:O  | 2.46                     | 0.57              |
| 1:B:216:UNK:C  | 1:B:218:UNK:N  | 2.64                     | 0.57              |
| 2:C:261:UNK:C  | 2:C:261:UNK:N  | 2.66                     | 0.57              |
| 1:A:136:UNK:C  | 1:A:262:UNK:O  | 2.48                     | 0.57              |
| 1:B:195:UNK:C  | 1:B:196:UNK:C  | 2.83                     | 0.57              |
| 1:A:120:UNK:C  | 1:A:121:UNK:O  | 2.46                     | 0.56              |
| 1:A:223:UNK:O  | 1:A:224:UNK:C  | 2.53                     | 0.56              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:232:UNK:O  | 1:A:235:UNK:N  | 2.39                     | 0.56              |
| 2:C:85:UNK:O   | 2:C:92:UNK:N   | 2.39                     | 0.56              |
| 1:A:267:UNK:CA | 1:A:267:UNK:O  | 2.41                     | 0.56              |
| 1:B:99:UNK:N   | 1:B:257:UNK:O  | 2.39                     | 0.56              |
| 1:B:158:UNK:N  | 1:B:242:UNK:O  | 2.39                     | 0.56              |
| 2:C:271:UNK:O  | 2:C:274:UNK:N  | 2.39                     | 0.56              |
| 1:B:124:UNK:O  | 1:B:128:UNK:N  | 2.39                     | 0.56              |
| 2:C:245:UNK:N  | 2:C:245:UNK:C  | 2.64                     | 0.55              |
| 1:B:197:UNK:C  | 1:B:198:UNK:CA | 2.77                     | 0.55              |
| 2:C:226:UNK:O  | 2:C:227:UNK:C  | 2.53                     | 0.55              |
| 1:A:195:UNK:O  | 1:A:196:UNK:C  | 2.55                     | 0.55              |
| 1:A:153:UNK:O  | 1:A:185:UNK:CA | 2.55                     | 0.55              |
| 1:B:95:UNK:N   | 1:B:95:UNK:O   | 2.39                     | 0.55              |
| 2:C:175:UNK:N  | 2:C:176:UNK:N  | 2.55                     | 0.54              |
| 2:C:234:UNK:C  | 2:C:235:UNK:CA | 2.79                     | 0.54              |
| 2:C:133:UNK:O  | 2:C:266:UNK:CA | 2.55                     | 0.54              |
| 2:C:229:UNK:CA | 2:C:230:UNK:N  | 2.66                     | 0.54              |
| 2:C:148:UNK:C  | 2:C:150:UNK:N  | 2.64                     | 0.54              |
| 2:C:235:UNK:CA | 2:C:235:UNK:O  | 2.37                     | 0.54              |
| 1:A:245:UNK:C  | 1:A:245:UNK:N  | 2.64                     | 0.54              |
| 1:B:177:UNK:CA | 2:C:268:UNK:O  | 2.55                     | 0.54              |
| 2:C:270:UNK:O  | 2:C:271:UNK:C  | 2.55                     | 0.54              |
| 1:A:171:UNK:O  | 1:A:172:UNK:C  | 2.55                     | 0.54              |
| 1:B:99:UNK:CA  | 1:B:257:UNK:O  | 2.55                     | 0.54              |
| 1:A:226:UNK:O  | 1:A:227:UNK:C  | 2.55                     | 0.54              |
| 1:B:110:UNK:N  | 1:B:110:UNK:C  | 2.60                     | 0.53              |
| 1:A:190:UNK:O  | 1:A:191:UNK:O  | 2.27                     | 0.53              |
| 1:A:193:UNK:O  | 1:A:198:UNK:N  | 2.41                     | 0.53              |
| 1:B:190:UNK:O  | 1:B:191:UNK:O  | 2.27                     | 0.53              |
| 1:A:111:UNK:N  | 1:A:243:UNK:O  | 2.41                     | 0.53              |
| 1:B:132:UNK:N  | 1:B:267:UNK:O  | 2.41                     | 0.53              |
| 2:C:201:UNK:CA | 2:C:201:UNK:O  | 2.48                     | 0.53              |
| 2:C:223:UNK:O  | 2:C:224:UNK:O  | 2.27                     | 0.53              |
| 2:C:81:UNK:C   | 2:C:82:UNK:CA  | 2.79                     | 0.53              |
| 1:B:270:UNK:O  | 1:B:271:UNK:C  | 2.55                     | 0.52              |
| 2:C:192:UNK:O  | 2:C:196:UNK:N  | 2.41                     | 0.52              |
| 1:B:201:UNK:CA | 1:B:202:UNK:N  | 2.57                     | 0.52              |
| 1:A:177:UNK:O  | 1:A:178:UNK:C  | 2.57                     | 0.52              |
| 1:B:198:UNK:C  | 1:B:200:UNK:N  | 2.73                     | 0.52              |
| 1:A:231:UNK:N  | 1:A:231:UNK:C  | 2.70                     | 0.52              |
| 2:C:210:UNK:C  | 2:C:210:UNK:N  | 2.66                     | 0.51              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:B:209:UNK:C  | 1:B:210:UNK:CA | 2.77                     | 0.51              |
| 1:B:162:UNK:C  | 1:B:163:UNK:CA | 2.66                     | 0.51              |
| 2:C:235:UNK:C  | 2:C:235:UNK:N  | 2.73                     | 0.51              |
| 2:C:273:UNK:C  | 2:C:275:UNK:H2 | 2.13                     | 0.51              |
| 2:C:142:UNK:O  | 2:C:258:UNK:N  | 2.44                     | 0.51              |
| 2:C:213:UNK:O  | 2:C:214:UNK:O  | 2.29                     | 0.50              |
| 1:A:116:UNK:O  | 1:A:117:UNK:C  | 2.60                     | 0.50              |
| 1:B:206:UNK:C  | 1:B:206:UNK:N  | 2.64                     | 0.50              |
| 2:C:232:UNK:C  | 2:C:234:UNK:N  | 2.75                     | 0.50              |
| 2:C:233:UNK:C  | 2:C:233:UNK:N  | 2.60                     | 0.50              |
| 2:C:175:UNK:CA | 2:C:175:UNK:O  | 2.41                     | 0.50              |
| 2:C:213:UNK:O  | 2:C:214:UNK:C  | 2.60                     | 0.50              |
| 1:A:128:UNK:C  | 1:A:130:UNK:N  | 2.75                     | 0.50              |
| 2:C:131:UNK:CA | 2:C:131:UNK:O  | 2.48                     | 0.49              |
| 1:B:131:UNK:N  | 1:B:131:UNK:C  | 2.73                     | 0.49              |
| 1:B:226:UNK:O  | 1:B:227:UNK:C  | 2.60                     | 0.49              |
| 1:B:274:UNK:N  | 1:B:275:UNK:N  | 2.60                     | 0.49              |
| 1:A:123:UNK:O  | 1:A:124:UNK:C  | 2.60                     | 0.49              |
| 2:C:126:UNK:N  | 2:C:126:UNK:C  | 2.66                     | 0.49              |
| 1:A:273:UNK:C  | 1:A:274:UNK:C  | 2.91                     | 0.49              |
| 2:C:106:UNK:N  | 2:C:248:UNK:CA | 2.75                     | 0.49              |
| 1:B:128:UNK:O  | 1:B:131:UNK:N  | 2.46                     | 0.49              |
| 1:B:177:UNK:C  | 1:B:178:UNK:C  | 2.91                     | 0.49              |
| 1:B:270:UNK:CA | 1:B:270:UNK:O  | 2.46                     | 0.49              |
| 1:A:171:UNK:O  | 1:A:174:UNK:N  | 2.46                     | 0.49              |
| 1:A:227:UNK:O  | 1:A:228:UNK:C  | 2.60                     | 0.49              |
| 2:C:224:UNK:C  | 2:C:225:UNK:C  | 2.91                     | 0.49              |
| 1:B:125:UNK:N  | 1:B:125:UNK:C  | 2.64                     | 0.49              |
| 1:B:162:UNK:C  | 1:B:163:UNK:C  | 2.91                     | 0.49              |
| 1:B:186:UNK:O  | 1:B:188:UNK:N  | 2.46                     | 0.49              |
| 2:C:132:UNK:N  | 2:C:267:UNK:O  | 2.46                     | 0.49              |
| 2:C:232:UNK:C  | 2:C:233:UNK:C  | 2.91                     | 0.48              |
| 2:C:233:UNK:O  | 2:C:236:UNK:N  | 2.46                     | 0.48              |
| 1:A:191:UNK:O  | 1:A:192:UNK:C  | 2.48                     | 0.48              |
| 1:A:271:UNK:N  | 1:A:271:UNK:C  | 2.64                     | 0.48              |
| 2:C:162:UNK:C  | 2:C:164:UNK:N  | 2.77                     | 0.48              |
| 1:B:210:UNK:N  | 1:B:210:UNK:C  | 2.53                     | 0.48              |
| 2:C:180:UNK:CA | 2:C:181:UNK:N  | 2.66                     | 0.48              |
| 2:C:76:UNK:C   | 2:C:77:UNK:C   | 2.91                     | 0.48              |
| 1:A:162:UNK:C  | 1:A:163:UNK:C  | 2.91                     | 0.47              |
| 1:B:109:UNK:C  | 1:B:110:UNK:CA | 2.75                     | 0.47              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:B:166:UNK:C  | 1:B:167:UNK:C  | 2.93                     | 0.47              |
| 1:A:270:UNK:C  | 1:A:271:UNK:C  | 2.93                     | 0.47              |
| 1:A:245:UNK:CA | 1:A:245:UNK:O  | 2.48                     | 0.47              |
| 1:B:190:UNK:C  | 1:B:191:UNK:C  | 2.93                     | 0.46              |
| 1:A:162:UNK:O  | 1:A:164:UNK:N  | 2.48                     | 0.46              |
| 2:C:224:UNK:C  | 2:C:226:UNK:N  | 2.79                     | 0.46              |
| 1:A:104:UNK:CA | 1:A:252:UNK:CA | 2.93                     | 0.46              |
| 1:B:127:UNK:O  | 1:B:128:UNK:C  | 2.64                     | 0.46              |
| 1:A:271:UNK:O  | 1:A:274:UNK:CA | 2.64                     | 0.46              |
| 1:A:118:UNK:O  | 1:A:119:UNK:C  | 2.64                     | 0.45              |
| 1:B:233:UNK:C  | 1:B:235:UNK:N  | 2.66                     | 0.45              |
| 2:C:192:UNK:O  | 2:C:193:UNK:C  | 2.64                     | 0.45              |
| 2:C:233:UNK:N  | 2:C:234:UNK:N  | 2.64                     | 0.45              |
| 2:C:273:UNK:N  | 2:C:274:UNK:N  | 2.64                     | 0.45              |
| 1:A:129:UNK:O  | 1:A:271:UNK:CA | 2.64                     | 0.45              |
| 1:B:125:UNK:O  | 1:B:126:UNK:C  | 2.64                     | 0.45              |
| 1:A:274:UNK:CA | 1:A:275:UNK:N  | 2.66                     | 0.45              |
| 1:A:138:UNK:O  | 1:A:261:UNK:CA | 2.64                     | 0.45              |
| 1:A:162:UNK:O  | 1:A:163:UNK:C  | 2.64                     | 0.45              |
| 1:B:101:UNK:CA | 1:B:102:UNK:H  | 2.27                     | 0.44              |
| 1:A:216:UNK:C  | 1:A:217:UNK:C  | 2.91                     | 0.44              |
| 1:A:212:UNK:C  | 1:A:213:UNK:CA | 2.73                     | 0.44              |
| 1:B:129:UNK:C  | 1:B:131:UNK:N  | 2.73                     | 0.44              |
| 2:C:195:UNK:O  | 2:C:196:UNK:C  | 2.66                     | 0.44              |
| 2:C:210:UNK:O  | 2:C:213:UNK:CA | 2.66                     | 0.44              |
| 2:C:269:UNK:O  | 2:C:270:UNK:C  | 2.66                     | 0.44              |
| 1:A:174:UNK:C  | 1:A:176:UNK:N  | 2.81                     | 0.43              |
| 1:A:184:UNK:C  | 1:A:185:UNK:O  | 2.64                     | 0.43              |
| 1:B:195:UNK:O  | 1:B:196:UNK:C  | 2.66                     | 0.43              |
| 1:B:163:UNK:N  | 1:B:164:UNK:N  | 2.66                     | 0.43              |
| 2:C:77:UNK:N   | 2:C:77:UNK:C   | 2.64                     | 0.43              |
| 1:A:157:UNK:C  | 1:A:157:UNK:H  | 2.25                     | 0.42              |
| 1:A:191:UNK:CA | 1:A:192:UNK:N  | 2.66                     | 0.42              |
| 1:A:210:UNK:C  | 1:A:212:UNK:H  | 2.32                     | 0.42              |
| 1:B:201:UNK:C  | 1:B:201:UNK:N  | 2.66                     | 0.42              |
| 1:A:131:UNK:C  | 1:A:131:UNK:N  | 2.66                     | 0.42              |
| 1:B:179:UNK:N  | 1:B:179:UNK:C  | 2.64                     | 0.42              |
| 2:C:212:UNK:C  | 2:C:214:UNK:N  | 2.79                     | 0.42              |
| 1:B:162:UNK:O  | 1:B:165:UNK:N  | 2.53                     | 0.42              |
| 2:C:77:UNK:C   | 2:C:78:UNK:C   | 2.97                     | 0.42              |
| 1:B:151:UNK:O  | 1:B:152:UNK:C  | 2.66                     | 0.42              |

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| Atom-1         | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 2:C:147:UNK:O  | 2:C:148:UNK:C | 2.66                     | 0.42              |
| 1:A:273:UNK:O  | 1:A:275:UNK:N | 2.53                     | 0.42              |
| 1:B:133:UNK:CA | 1:B:134:UNK:N | 2.66                     | 0.42              |
| 1:B:164:UNK:O  | 1:B:165:UNK:C | 2.66                     | 0.42              |
| 2:C:114:UNK:O  | 2:C:116:UNK:N | 2.53                     | 0.42              |
| 1:A:173:UNK:C  | 1:A:174:UNK:C | 2.91                     | 0.41              |
| 1:A:194:UNK:N  | 1:A:195:UNK:N | 2.66                     | 0.41              |
| 1:B:192:UNK:O  | 1:B:195:UNK:N | 2.53                     | 0.41              |
| 1:A:210:UNK:C  | 1:A:212:UNK:N | 2.83                     | 0.41              |
| 1:A:157:UNK:O  | 1:A:157:UNK:N | 2.53                     | 0.40              |
| 1:B:229:UNK:N  | 1:B:229:UNK:C | 2.66                     | 0.40              |

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

#### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | C     | 29               |
| 1   | B     | 26               |
| 1   | A     | 22               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 186:UNK   | C      | 187:UNK   | N      | 1.66         |
| 1     | B     | 210:UNK   | C      | 211:UNK   | N      | 1.66         |
| 1     | C     | 236:UNK   | C      | 237:UNK   | N      | 1.66         |
| 1     | A     | 103:UNK   | C      | 104:UNK   | N      | 1.17         |
| 1     | A     | 141:UNK   | C      | 142:UNK   | N      | 1.17         |
| 1     | A     | 147:UNK   | C      | 148:UNK   | N      | 1.17         |
| 1     | B     | 149:UNK   | C      | 150:UNK   | N      | 1.17         |
| 1     | B     | 162:UNK   | C      | 163:UNK   | N      | 1.17         |
| 1     | B     | 202:UNK   | C      | 203:UNK   | N      | 1.17         |
| 1     | B     | 208:UNK   | C      | 209:UNK   | N      | 1.17         |
| 1     | B     | 228:UNK   | C      | 229:UNK   | N      | 1.17         |
| 1     | B     | 236:UNK   | C      | 237:UNK   | N      | 1.17         |
| 1     | C     | 135:UNK   | C      | 136:UNK   | N      | 1.17         |
| 1     | C     | 146:UNK   | C      | 147:UNK   | N      | 1.17         |
| 1     | C     | 158:UNK   | C      | 159:UNK   | N      | 1.17         |
| 1     | C     | 235:UNK   | C      | 236:UNK   | N      | 1.17         |
| 1     | C     | 241:UNK   | C      | 242:UNK   | N      | 1.17         |
| 1     | C     | 266:UNK   | C      | 267:UNK   | N      | 1.17         |
| 1     | A     | 95:UNK    | C      | 96:UNK    | N      | 1.12         |
| 1     | A     | 104:UNK   | C      | 105:UNK   | N      | 1.12         |
| 1     | A     | 108:UNK   | C      | 109:UNK   | N      | 1.12         |
| 1     | A     | 114:UNK   | C      | 115:UNK   | N      | 1.12         |
| 1     | A     | 119:UNK   | C      | 120:UNK   | N      | 1.12         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 136:UNK   | C      | 137:UNK   | N      | 1.12         |
| 1     | A     | 144:UNK   | C      | 145:UNK   | N      | 1.12         |
| 1     | A     | 171:UNK   | C      | 172:UNK   | N      | 1.12         |
| 1     | B     | 155:UNK   | C      | 156:UNK   | N      | 1.12         |
| 1     | B     | 183:UNK   | C      | 184:UNK   | N      | 1.12         |
| 1     | B     | 195:UNK   | C      | 196:UNK   | N      | 1.12         |
| 1     | B     | 218:UNK   | C      | 219:UNK   | N      | 1.12         |
| 1     | B     | 225:UNK   | C      | 226:UNK   | N      | 1.12         |
| 1     | B     | 233:UNK   | C      | 234:UNK   | N      | 1.12         |
| 1     | B     | 247:UNK   | C      | 248:UNK   | N      | 1.12         |
| 1     | B     | 248:UNK   | C      | 249:UNK   | N      | 1.12         |
| 1     | C     | 93:UNK    | C      | 94:UNK    | N      | 1.12         |
| 1     | C     | 105:UNK   | C      | 106:UNK   | N      | 1.12         |
| 1     | C     | 108:UNK   | C      | 109:UNK   | N      | 1.12         |
| 1     | C     | 115:UNK   | C      | 116:UNK   | N      | 1.12         |
| 1     | C     | 116:UNK   | C      | 117:UNK   | N      | 1.12         |
| 1     | C     | 152:UNK   | C      | 153:UNK   | N      | 1.12         |
| 1     | C     | 165:UNK   | C      | 166:UNK   | N      | 1.12         |
| 1     | C     | 175:UNK   | C      | 176:UNK   | N      | 1.12         |
| 1     | C     | 195:UNK   | C      | 196:UNK   | N      | 1.12         |
| 1     | C     | 215:UNK   | C      | 216:UNK   | N      | 1.12         |
| 1     | C     | 231:UNK   | C      | 232:UNK   | N      | 1.12         |
| 1     | C     | 239:UNK   | C      | 240:UNK   | N      | 1.12         |
| 1     | C     | 248:UNK   | C      | 249:UNK   | N      | 1.12         |
| 1     | C     | 272:UNK   | C      | 273:UNK   | N      | 1.12         |
| 1     | A     | 106:UNK   | C      | 107:UNK   | N      | 1.07         |
| 1     | A     | 109:UNK   | C      | 110:UNK   | N      | 1.07         |
| 1     | A     | 131:UNK   | C      | 132:UNK   | N      | 1.07         |
| 1     | A     | 217:UNK   | C      | 218:UNK   | N      | 1.07         |
| 1     | A     | 247:UNK   | C      | 248:UNK   | N      | 1.07         |
| 1     | B     | 99:UNK    | C      | 100:UNK   | N      | 1.07         |
| 1     | B     | 140:UNK   | C      | 141:UNK   | N      | 1.07         |
| 1     | B     | 141:UNK   | C      | 142:UNK   | N      | 1.07         |
| 1     | B     | 163:UNK   | C      | 164:UNK   | N      | 1.07         |
| 1     | B     | 190:UNK   | C      | 191:UNK   | N      | 1.07         |
| 1     | B     | 246:UNK   | C      | 247:UNK   | N      | 1.07         |
| 1     | B     | 255:UNK   | C      | 256:UNK   | N      | 1.07         |
| 1     | B     | 265:UNK   | C      | 266:UNK   | N      | 1.07         |
| 1     | C     | 198:UNK   | C      | 199:UNK   | N      | 1.07         |
| 1     | C     | 225:UNK   | C      | 226:UNK   | N      | 1.07         |
| 1     | C     | 263:UNK   | C      | 264:UNK   | N      | 1.07         |
| 1     | A     | 129:UNK   | C      | 130:UNK   | N      | 1.01         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 139:UNK   | C      | 140:UNK   | N      | 1.01         |
| 1     | A     | 194:UNK   | C      | 195:UNK   | N      | 1.01         |
| 1     | A     | 230:UNK   | C      | 231:UNK   | N      | 1.01         |
| 1     | B     | 128:UNK   | C      | 129:UNK   | N      | 1.01         |
| 1     | B     | 219:UNK   | C      | 220:UNK   | N      | 1.01         |
| 1     | B     | 232:UNK   | C      | 233:UNK   | N      | 1.01         |
| 1     | C     | 134:UNK   | C      | 135:UNK   | N      | 1.01         |
| 1     | C     | 174:UNK   | C      | 175:UNK   | N      | 1.01         |
| 1     | C     | 213:UNK   | C      | 214:UNK   | N      | 1.01         |
| 1     | C     | 218:UNK   | C      | 219:UNK   | N      | 1.01         |
| 1     | C     | 261:UNK   | C      | 262:UNK   | N      | 1.01         |
| 1     | A     | 225:UNK   | C      | 226:UNK   | N      | 0.96         |

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.